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Computational Screening toward Transition Metal Doped VC in Different Crystal Planes for Efficient Hydrogen Evolution: A First-Principles Study

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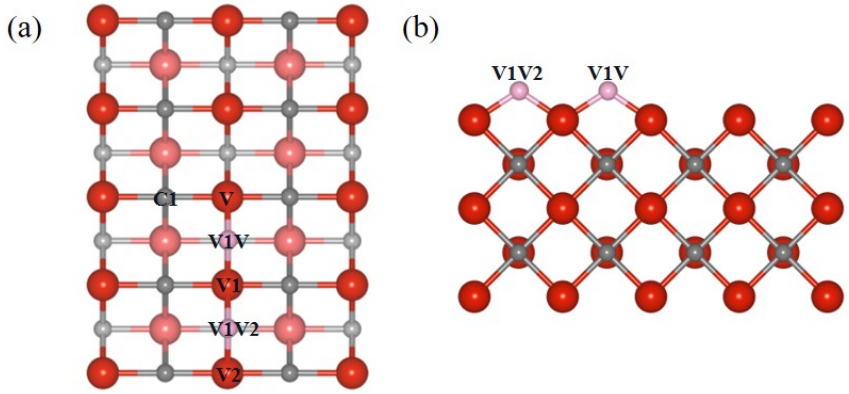

Fig. S1 The location of the bridge-active sites on the VC(110) model. (a) Top view. (b) Side view. The red, grey, and pink balls in the ball-stick models indicated V, C, and H atoms.

Tab. S1 The values of ZPE, ΔZPE, ΔE_{H^*}, and ΔG_{H^*} of hydrogen atoms at the different adsorption sites of TM-VC (100).

(100)	ZPE1	ZPE2	ZPE3	ΔZPE	ΔE_{H^*}	ΔG_{H^*}
VC C site	340.4228	27.4093	25.5601	0.1967	-0.0811	0.1801
VC V site	321.5908	62.1226	0	0.1919	0.5448	0.8012
Co-VC Co site	326.0123	71.4440	0	0.1987	0.438	0.7012
Co-VC V site	200.8555	56.2845	54.8995	0.1560	0.5913	0.8118
Co-VC C site	347.0149	57.1230	38.9784	0.2216	-0.5371	-0.2510
Fe-VC Fe site	240.1155	70.1219	61.3435	0.1858	0.4033	0.6536
Fe-VC V site	205.4249	82.9177	0	0.1442	0.5910	0.7997
Fe-VC C site	355.9924	28.2529	0	1.1921	-0.3053	-0.0487
Ni-VC Ni site	249.1690	112.0342	63.1592	0.2122	0.7583	1.0349
Ni-VC V site	338.1450	57.9366	0	0.1980	0.6216	0.8842
Ni-VC C site	345.3871	61.0862	40.7997	0.2236	-0.4577	-0.1695
Mn-VC Mn site	226.3255	70.2720	69.8436	0.1832	0.3813	0.6290
Mn-VC V site	249.3710	95.3077	0	0.1723	0.5872	0.8240
Mn-VC C site	342.7514	56.7085	28.8076	0.2141	-0.2775	0.0012
Mo-VC Mo site	240.8132	84.4082	0	0.1626	0.2779	0.5050
Mo-VC V site	230.9060	64.3921	0	0.1476	0.5317	0.7439
Mo-VC C site	350.2801	29.0889	0	0.1897	-0.1410	0.1132

Tab. S2 The values of ZPE, ΔZPE, ΔE_{H^*}, and ΔG_{H^*} of hydrogen atoms at the different adsorption sites of TM-VC (110).

(110)	ZPE1	ZPE2	ZPE3	ΔZPE	ΔE_{H^*}	ΔG_{H^*}
VC bridge V_1V site	150.3009	146.9175	57.0462	0.1771	-0.3367	-0.0950
VC C site	348.8280	77.2670	46.1616	0.2361	-1.0526	-0.7519
VC V site	198.8634	16.1405	0	0.1075	0.2559	0.4279
Co-VC C site	364.2330	90.9773	76.8920	0.2661	-1.2899	-0.9593
Co-VC Co site	230.8826	56.6804	0	0.1438	-0.0917	0.1166
Co-VC bridge V_1V_2 site	153.5855	139.4671	59.9405	0.1765	-0.2722	-0.0312
Co-VC V site	201.1082	39.5432	0	0.1203	0.2587	0.4435
Co-VC bridge V_1Co site	186.9527	85.5654	0	0.1363	-0.1861	0.0146
Fe-VC C site	354.3472	76.2572	65.4422	0.2480	-1.2516	-0.9391
Fe-VC Fe site	228.6672	63.5080	0	0.1461	-0.1740	0.0366
Fe-VC bridge V_1V_2 site	151.4732	141.7359	60.5419	0.1769	-0.2807	-0.0393
Fe-VC V site	199.3281	37.9594	0	0.1186	0.2550	0.4381
Fe-VC bridge V_1Fe site	182.6690	89.9685	70.7778	0.1717	-0.2571	-0.0209
Ni-VC C site	361.7385	77.3231	0	0.2195	-1.2773	-0.9932
Ni-VC Ni site	229.8686	36.9447	0	0.1334	0.1656	0.3635
Ni-VC bridge V_1V_2 site	171.8235	151.6687	0	0.1617	-0.2478	-0.0215
Ni-VC V site	276.5147	0	0	0.1383	0.2757	0.4785
Ni-VC bridge V_1Ni site	166.8327	97.5119	63.2317	0.1638	-0.0140	0.2142
Mn-VC C site	352.1259	77.3882	65.2584	0.2474	-1.2095	-0.8977
Mn-VC Mn site	231.1138	0	0	0.1156	-0.0718	0.1083
Mn-VC bridge V_1V_2 site	149.8111	141.5312	61.4604	0.1764	-0.2985	-0.0576
Mn-VC V site	199.5333	37.0897	0	0.1183	0.2564	0.4392
Mn-VC bridge V_1Mn site	160.8185	119.6245	67.3553	0.1739	-0.2566	-0.0182
Mo-VC C site	338.9793	74.0891	60.9111	0.2370	-0.9529	-0.6514
Mo-VC Mo site	209.8593	60.7097	0	0.1353	0.0112	0.2110
Mo-VC bridge V_1V_2 site	147.8526	145.8331	60.1527	0.1769	-0.3287	-0.0873
Mo-VC V site	199.0872	21.3336	0	0.1102	0.2530	0.4277
Mo-VC bridge V_1Mo site	155.0415	139.1191	62.3088	0.1782	-0.3974	-0.1546

Tab. S3 The values of ZPE, ΔZPE, ΔE_{H^*}, and ΔG_{H^*} of hydrogen atoms at the different adsorption sites of TM-VC (111).

(111)	ZPE1	ZPE2	ZPE3	ΔZPE	ΔE_{H^*}	ΔG_{H^*}
VC V site	192.6112	41.6851	0	0.1171	-0.0564	0.1253
VC C site	148.1868	85.8038	52.4867	0.1432	-0.9053	-0.6976
Co-VC Co site	228.0789	22.3464	0	0.1252	-0.4289	-0.2392
Co-VC C site	158.0140	49.3818	0	0.1037	-0.5108	-0.3426
Co-VC V site	192.7189	19.6462	0	0.1062	-0.0906	0.0801
Fe-VC Fe site	225.3897	24.4790	22.5929	0.1362	-0.5234	-0.3226
Fe-VC C site	136.9755	78.4136	50.4681	0.1329	-0.5679	-0.3705
Fe-VC V site	191.2509	0	0	0.0956	-0.0771	0.0830
Ni-VC Ni site	225.4188	0	0	0.1127	-0.1383	0.0389
Ni-VC V site	187.3990	0	0	0.0937	-0.0944	0.0638
Mn-VC Mn site	220.7717	35.4944	27.4304	0.1418	-0.4186	-0.2123
Mn-VC C site	151.8739	73.6433	0	0.1127	-0.6637	-0.4864
Mn-VC V site	190.6365	54.5928	0	0.1226	-0.0691	0.1180
Mo-VC Mo site	211.3261	41.4017	20.4216	0.1366	-0.3415	-0.1404
Mo-VC V site	190.2645	0	0	0.0951	-0.0184	0.1412
Mo-VC C site	140.9009	89.4241	76.8064	0.1536	-0.9365	-0.7184